Ethylene oxide 75-21-8 | DTXSID0020600

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 860 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.01e-01

Confidence level: 8.00e-01

Nearest Neighbors from the Training Set

Image not found

Cyclopropane Measured: 1310 Predicted: 3500 Image not found

Azetidine

Measured: 324 Predicted: 155 Image not found

1,1-Dichloroethylene Measured: 538 Predicted: 282

Image not found

Glyoxal Measured

Measured: 1320 Predicted: 128 Image not found

Diethylamine Measured: 511 Predicted: 134